Time-Dependent Density-Functional Theory for Trapped Strongly-Interacting Fermionic Atoms

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The dynamics of strongly interacting trapped dilute Fermi gases (dilute in the sense that the range of interatomic potential is small compared with inter-particle spacing) is investigated in a single-equation approach to the time-dependent density-functional theory. Our results are in good agreement with recent experimental data in the BCS-BEC crossover regime.

It is also shown that the calculated corrections to the hydrodynamic approximation may be important even for systems with a rather large number of atoms.

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The recently reported ultracold trapped Fermi gases with tunable atomic scattering length [1-11] in the vicinity of a Feshbach resonance stimulated a large number of theoretical investigations. Some of these works are based on the assumption that the properties of strongly interacting dilute Fermi gas at zero temperature are well described by the hydrodynamic approximation (HA) [12-15]

$$\frac{\partial n}{\partial t} + \nabla(n\vec{\mathrm{v}}) = 0, \tag{1}$$

$$\frac{\partial \vec{\mathrm{v}}}{\partial t} + \frac{1}{m}\nabla(V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n} + \frac{1}{2}m\mathrm{v}^2) = 0, \tag{2}$$

where n is the density, $\epsilon(n)$ is the ground-state energy per particle of the homogeneous system and $\vec{\mathrm{v}}$ is the velocity field.

In this paper the dynamics of strongly interacting trapped dilute Fermi gases (dilute in the sense that the range of interatomic potential is small compared with inter-particle spacing) is investigated in the single equation approach to the time-dependent density-functional theory covering the whole crossover region at zero temperature. It is shown for the case of elongated cigar-shaped harmonic traps that the calculated corrections to the HA may be important even for systems with a rather large number of atoms.

We mention here Refs.[16] where an extension of the density-functional theory (DFT) to superconducting systems [17] was generalized to a number of nuclear and atomic systems.

Let us consider a Fermi gas consisting of a 50-50 mixture of two different states confined in a harmonic trap $V_{ext}(\vec{r}) = (m/2)(\omega_\perp^2(x^2+y^2) + \omega_z^2 z^2)$. In Eq.(2), the kinetic-energy density $t(n)$ is approximated by the Thomas-Fermi (TF) kinetic-energy density $t_{TF}(n) = (3/10)n\hbar^2 k_F^2/m$, where $k_F = (3\pi^2 n)^{1/3}$. For slowly varying densities characterized by the condition $\mid \nabla n \mid /n^{4/3} \ll 1$, the kinetic energy density is well represented by the Kirzhnitz gradient expansion (KGE) [18] $t(n) = t_{TF}(n) + t_W(n)/9 + ...$, where $t_W(n) = (\hbar^2/(8m))(\nabla n)^2/n$ is the original von Weizsäcker density (OWD)[19], which gives the entire kinetic energy density of noninteracting bosons.

In the case of large but finite number of atoms N, the density n is not constant. At small distances the ratio $\mid \nabla n \mid /n^{4/3}$ is small and both the Kirzhnitz correction and the OWD are negligible. On the contrary, near the surface the Hartree-Fock (HF) type densities are proportional to the square of the last occupied state. Therefore, the OWD is important in this case and it is expected to determine the asymptotic behavior of the density at large

distances. It is also expected that the OWD is important in the case of the tight radial trapping, $\lambda \ll 1$. In Refs.[20], the OWD was considered as a correction to the TF kinetic-energy density.

Adding the OWD to $t_{TF}(n)$ we have

$$\frac{\partial \vec{\mathrm{v}}}{\partial t} + \frac{1}{m}\nabla(V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n} + \frac{1}{2}m\mathrm{v}^2 - \frac{\hbar^2}{2m}\frac{1}{\sqrt{n}}\nabla^2\sqrt{n}) = 0. \tag{3}$$

We define the density of the system as $n(\vec{r},t) = \mid \Psi(\vec{r},t) \mid^2$, and the velocity field $\vec{\mathrm{v}}$ as $\vec{\mathrm{v}}(\vec{r},t) = \hbar(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*)/(2imn(\vec{r},t))$. From Eqs.(1) and (3), we obtain the following nonlinear Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V_{ext}\Psi + \frac{\partial(n\epsilon(n))}{\partial n}\Psi, \tag{4}$$

which is equivalent, to a certain extent, to the single equation approach of Deb et al. [21] to the time-dependent density-functional theory (TDDFT).

If the trap potential, V_{ext}, is independent of time, one can write $\Psi(\vec{r},t) = \Phi(\vec{r})\exp(-i\mu t/\hbar)$, where μ is the chemical potential, and Φ is normalized to the total number of particles, $\int d\vec{r} \mid \Phi \mid^2 = N$. Then Eq.(4) becomes

$$(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext} + \frac{\partial(n\epsilon(n))}{\partial n})\Phi = \mu\Phi, \tag{5}$$

where the solution of the equation (5) minimizes the energy functional $E = N < \Phi \mid -\frac{\hbar^2}{2m}\nabla^2 + V_{ext} + \epsilon(n) \mid \Phi >$, and the chemical potential μ is given by $\mu = \partial E/\partial N$.

In order to take into account atoms lost by inelastic collisions, we model the loss by the rate equation

$$\frac{dN}{dt} = -\int \chi(\vec{r},t)d\vec{r},$$

where $\chi(\vec{r},t) = \sum_{l=1} k_l n^l g_l(n)$, $n^l g_l$ is the local l-particle correlation function and k_l is the rate constant for the l-body atoms loss. The generalization of Eq.(4) for the case of inelastic collisions reads [22]

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V_{ext}\Psi + \frac{\partial(n\epsilon(n))}{\partial n}\Psi - i\frac{\hbar}{2}\sum_{l=1} k_l n^{l-1} g_l(n)\Psi. \tag{6}$$

For the negative S-wave scattering length between the two fermionic species, $a < 0$, in the low-density regime, $k_F \mid a \mid \ll 1$, the ground state energy per particle , $\epsilon(n)$, is well represented by an expansion in power of $k_F \mid a \mid$ [26]

$$\epsilon(n) = 2E_F[\frac{3}{10} - \frac{1}{3\pi}k_F \mid a \mid + 0.055661(k_F \mid a \mid)^2 - 0.00914(k_F \mid a \mid)^3 + ...], \tag{7}$$

where $E_F = \hbar^2 k_F^2/(2m)$. In the opposite regime, $a \to -\infty$ (the Bertsch many-body problem, quoted in Refs.[27]), $\epsilon(n)$ is proportional to that of the non-interacting Fermi gas

$$\epsilon(n) = (1+\beta)\frac{3}{10}\frac{\hbar^2 k_F^2}{m}, \tag{8}$$

where a universal parameter β is estimated to be $\beta = -0.56$ [28].

In the $a \to +0$ limit the system reduces to the dilute Bose gas of dimers [29]

$$\epsilon(n) = E_F(-1/(k_F a)^2 + a_m k_F/(6\pi) + ...,) \tag{9}$$

where a_m is the boson-boson scattering length. While the BCS mean-field theories [30] predict $a_m = 2a$ [31], a solution of 4-fermion problem for contact scattering provided the value $a_m \approx 0.6a$ [32].

Very little is known about the correct form of $\epsilon(n)$ in the intermediate range. Therefore, a simple interpolation of the form $\epsilon(n) \approx E_F P(k_F a)$ with a smooth function $P(x)$ mediating between the known limits suggests itself as a pragmatic alternative.

In Ref.[33] it has been proposed a [2/2] Padé approximant for the function $P(x)$ for the negative a

$$P(x) = \frac{3}{5} - 2\frac{\delta_1 \mid x \mid + \delta_2 x^2}{1 + \delta_3 \mid x \mid + \delta_4 x^2}, \tag{10}$$

where $\delta_1 = 0.106103$, $\delta_2 = 0.187515$, $\delta_3 = 2.29188$, $\delta_4 = 1.11616$. Eq.(10) is constructed to reproduce the first four terms of the expansion (6) in the low-density regime and also to reproduce exactly results of the recent Monte Carlo calculations [28], $\beta = -0.56$, in the unitary limit, $k_F a \to -\infty$.

For the positive a case (the interaction is strong enough to form bound molecules with energy E_{mol}) we consider a [2/2] Padé approximant

$$P(x) = \frac{E_{mol}}{2E_F} + \frac{\alpha_1 x + \alpha_2 x^2}{1 + \alpha_3 x + \alpha_4 x^2}, \tag{11}$$

where parameters α are fixed by two continuity conditions at large x, $1/x \to 0$, and by two continuity conditions at small x. For example, $\alpha_1 = 0.0316621$, $\alpha_2 = 0.0111816$, $\alpha_3 = 0.200149$, and $\alpha_4 = 0.0423545$ for $a_m = 0.6a$.

Fig. 1 and Fig. 2 show the comparison between [2/2] Padé approximations, Eqs.(10,11), and the lowest order constrained variational (LOCV) approximation [34] and the BCS mean-field theory for $\epsilon(n)$. The LOCV calculations agree very well with the [2/2] Pade approximation results on the BCS side ($a < 0$). It is evident the difference between our results and

the BCS mean-field theory calculations. For example, the BCS mean-field gives $\beta = -0.41$. We mention here that $\epsilon(n)/E_F$ on the BCS side ($a < 0$) and $(\epsilon(n) + |E_{mol}|/2)/E_F$ on the BEC side ($a > 0$) show a smooth monotonic behavior as a function of $k_F a$.

The predictions of Eq.(5) with $\epsilon(n)$ from Eq.(10) for the axial cloud size of strongly interacting ^6Li atoms are shown in Fig 3 [35]. It indicates that the TF approximation of the kinetic energy density is a very good approximation for the experimental conditions of Ref.[11], $N\lambda \approx 10^4$ (inclusion of the OWD gives a negligible effect, $< 0.5\%$) [37].

It can be proved [24] that every solution of equation (4) is a stationary point of an action corresponding to the Lagrangian density

$$\mathcal{L}_0 = \frac{i\hbar}{2}(\Psi\frac{\partial\Psi^*}{\partial t} - \Psi^*\frac{\partial\Psi}{\partial t}) + \frac{\hbar^2}{2m} \mid \nabla\Psi \mid^2 + \epsilon(n)n + V_{ext}n,$$

which for $\Psi = e^{i\phi(\vec{r},t)}n^{1/2}(\vec{r},t)$ can be rewritten as

$$\mathcal{L}_0 = \hbar\dot{\phi}n + \frac{\hbar^2}{2m}(\nabla\sqrt{n})^2 + \frac{\hbar^2}{2m}n(\nabla\phi)^2 + \epsilon(n)n + V_{ext}n.$$

For a time-dependent harmonic trap, $V_{ext}(\vec{r},t) = (m/2)\sum_{i=1}^{3}\omega_i^2(t)x_i^2$, a suitable trial function can be taken as $\phi(\vec{r},t) = \chi(t) + (m/(2\hbar)\sum_{i=1}^{3}\eta_i(t)x_i^2$, $n(\vec{r},t) = n_0(x_i/b_i(t))/\zeta(t)$, where $\zeta(t) = \prod_j b_j$. With this ansatz, the Hamilton principle, $\delta\int dt\int\mathcal{L}_0 d^3r = 0$, gives the following equations for the scaling parameters b_i

$$\ddot{b}_i + \omega_i^2(t)b_i - \frac{2 < T_i >}{m < x_i^2 > b_i^3} - \frac{1}{m < x_i^2 > b_i}\int [n^2 d\epsilon(n)/dn]_{n=n_0(\vec{r})/\zeta(t)}d^3r\zeta(t) = 0, \qquad (12)$$

where $b_i(0) = 1$, $\dot{b}_i(0) = 0$ and $\omega_i = \omega_i(0)$ fix the initial configuration of the system, corresponding to the density $n_0(\vec{r})$ and $< T_i >= -\hbar^2/(2mN)\int n^{1/2}(\partial^2/\partial x_i^2)n^{1/2}d^3r$, $< x_i^2 >= (1/N)\int nx_i^2 d^3r$.

Expanding Eqs.(12) around equilibrium ($b_i = 1$) we get the following equations for the collective frequencies, ω

$$(2 + \kappa_i - \frac{\omega^2}{\omega_i^2})y_i + (1 + \frac{1}{2}\kappa_i + \chi_i)(y_1 + y_2 + y_3) = 0, \qquad (13)$$

where $\kappa_i = 4 < T_i > /(m\omega_i^2 < x_i^2 >)$ and $\chi_i = \int n_0^3\partial^2\epsilon/(\partial n_0^2)d^3r/(m\omega_i^2 < x_i^2 >)$.

In Table I we give the calculated values of the radial breathing mode frequency, $\nu = \omega_{rad}/(2\pi)$, of highly degenerate gas of ^6Li atoms near a Feshbach resonance at 822 G [41]. It can be seen from Table I, that the difference between two approximations, Eqs.(1,2)

and Eq.(4), is less than 0.75%, and both approximations give a very good agreement with experimental data of Ref.[1]. The parameter λN for this case is very large, $\lambda N \geq 10^4$.

In Fig. 4, we present the calculations for the frequency of the radial compression mode ω_{rad} as a function of the dimensional parameter $(N^{1/6}a/a_{ho})^{-1}$ in the case of an anisotropic trap ($\omega_x = \omega_y = \omega_\perp$, $\omega_z/\omega_\perp = \lambda$). One can easily see that the corrections to the hydrodynamic approximation (HA), Eqs.(1) and (2), are important even for relatively large N and λN. For example, the correction to ω_{rad} in unitary limit is larger than 11% and 25% for $\lambda = 10^{-2}$, $N = 10^4$ and $\lambda = 10^{-2}$, $N = 10^3$, respectively.

In the HA, ω_{rad} is independent of N for a fixed $(N^{1/6}a/a_{ho})^{-1}$. The deviation from this behavior does not demonstrate the cross-over to the $1D$ behavior, since $\lambda N > 1$ [42]. It demonstrates that the validity of the HA depends on the properties of the trap. In Ref.[43] it was shown that, for the case of isotropic trap, $\lambda = 1$, with $N = 20$ and $N = 240$, the TF approximation reproduces the energy within accuracies of 2% and 1%, respectively.

In Fig.5, the calculated radial compressional frequency is compared with experimental data [1] in the BCS-BEC crossover region. There is a very good agreement between calculations and experimental data [1]. However our calculations for ω_{rad} disagree with experimental data of Ref.[44].

In the present paper, we have used Eq.(4). The next step is to develop the Kohn-Sham time-dependent DFT [45] for two-component Fermi gases in elongated traps ($\lambda \ll 1$), which we will consider in our future work.

In conclusion, the dynamics of strongly interacting trapped dilute Fermi gases is investigated in the single equation approach to the time-dependent density-functional theory. Our results are in good agreement with recent experimental data in the BCS-BEC crossover regime.

It is also shown that the calculated corrections to the hydrodynamic approximation may be important even for systems with a rather large number of atoms.

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Note added. - While this work was being prepared for publication, preprints [46] appeared in which the authors calculate the equation of state, $\epsilon(n)$, using the quantum Monte Carlo method. Their results are in a good agreement with ours Padé [2/2] approximation for both negative and positive scattering length.

Table I. Radial breathing mode frequencies $\nu = \omega_{rad}/(2\pi)$ of highly degenerate gas of ^6Li atoms near a 822(G) Feshbach resonance [36]. B is applied magnetic field, ν_{exp} indicate experimental data from the Duke University group [1], ν and ν_{TF} represent theoretical calculations that use equation (4) and the hydrodynamic approximation (equations (1) and (2)), respectively. The trap parameters are $\omega_\perp = 2\pi \times 1549$, $\omega_z = 2\pi \times 70$.

$B(G)$	$N(10^3)$	ν_{exp}(Hz) [1]	ν(Hz)	ν_{TF}(Hz)
860	294	2857	2810	2793
870	288	2837	2804	2787
870	225	2838	2806	2786
870	379	2754	2803	2788
870	290	2775	2804	2787
870	244	2779	2805	2787
880	258	2836	2800	2783
910	268	2798	2792	2775

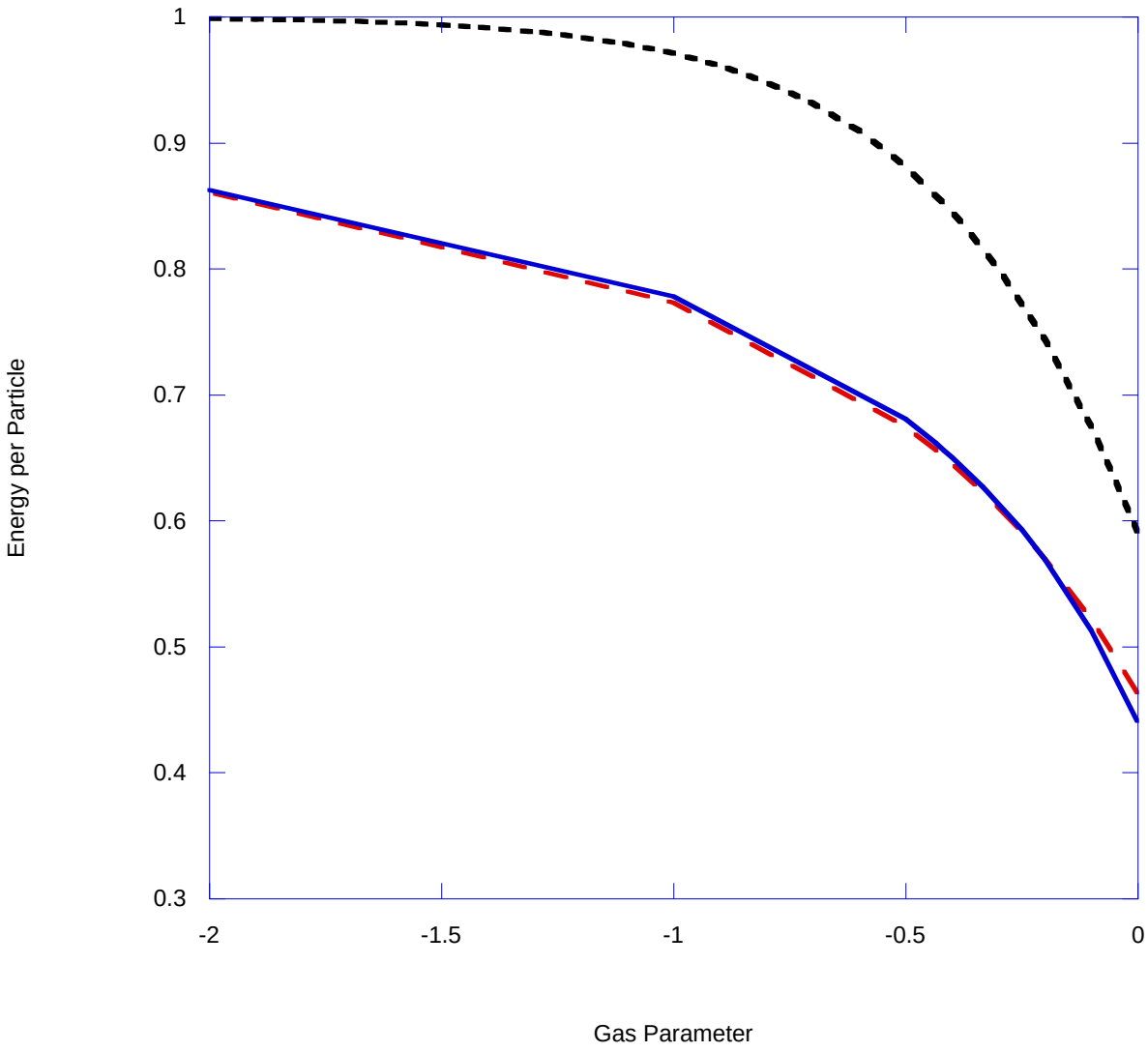

Fig.1. The ground state energy per particle, $\epsilon(n)$, in units of $3\hbar^2 k_F^2/(10m)$ as a function of the gas parameter $(k_F a)^{-1}$. The solid line, the long dashed line and the short dashed line represent the results calculated using the [2/2] Padé approximation, Eq.(10), the LOCV approximation, and the BCS mean-field theory, respectively.

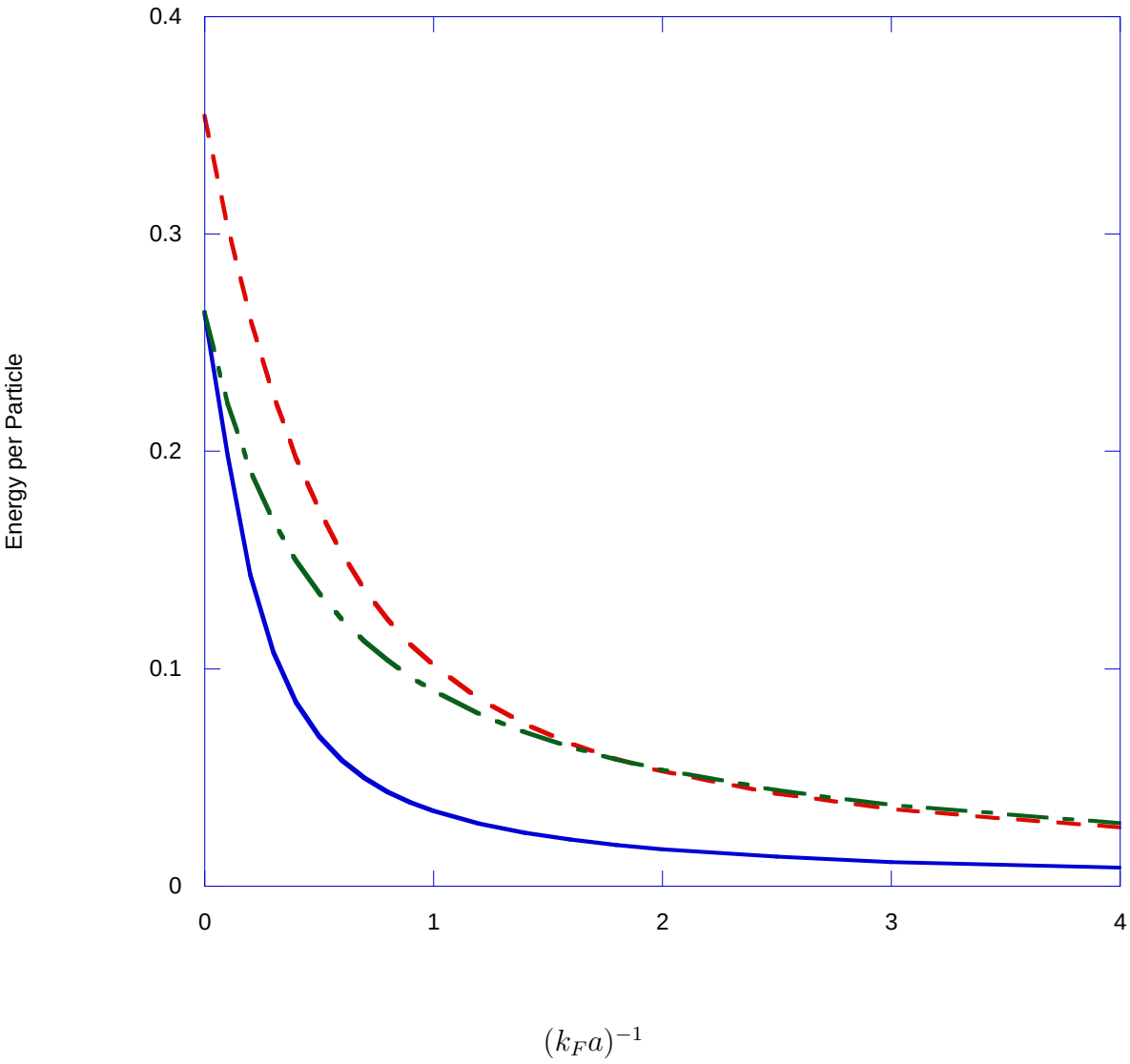

Fig.2. The ground state energy per particle, $\epsilon(n) + |E_{mol}|/2$, in units of $\hbar^2 k_F^2/(2m)$ as a function of the gas parameter $(k_F a)^{-1}$. The dashed line, the dotted-dashed line and the solid line represent the results calculated using the BCS mean-field theory, the [2/2] Padé approximation, Eq.(11), with $a_m = 2a$, and $a_m = 0.6a$, respectively.

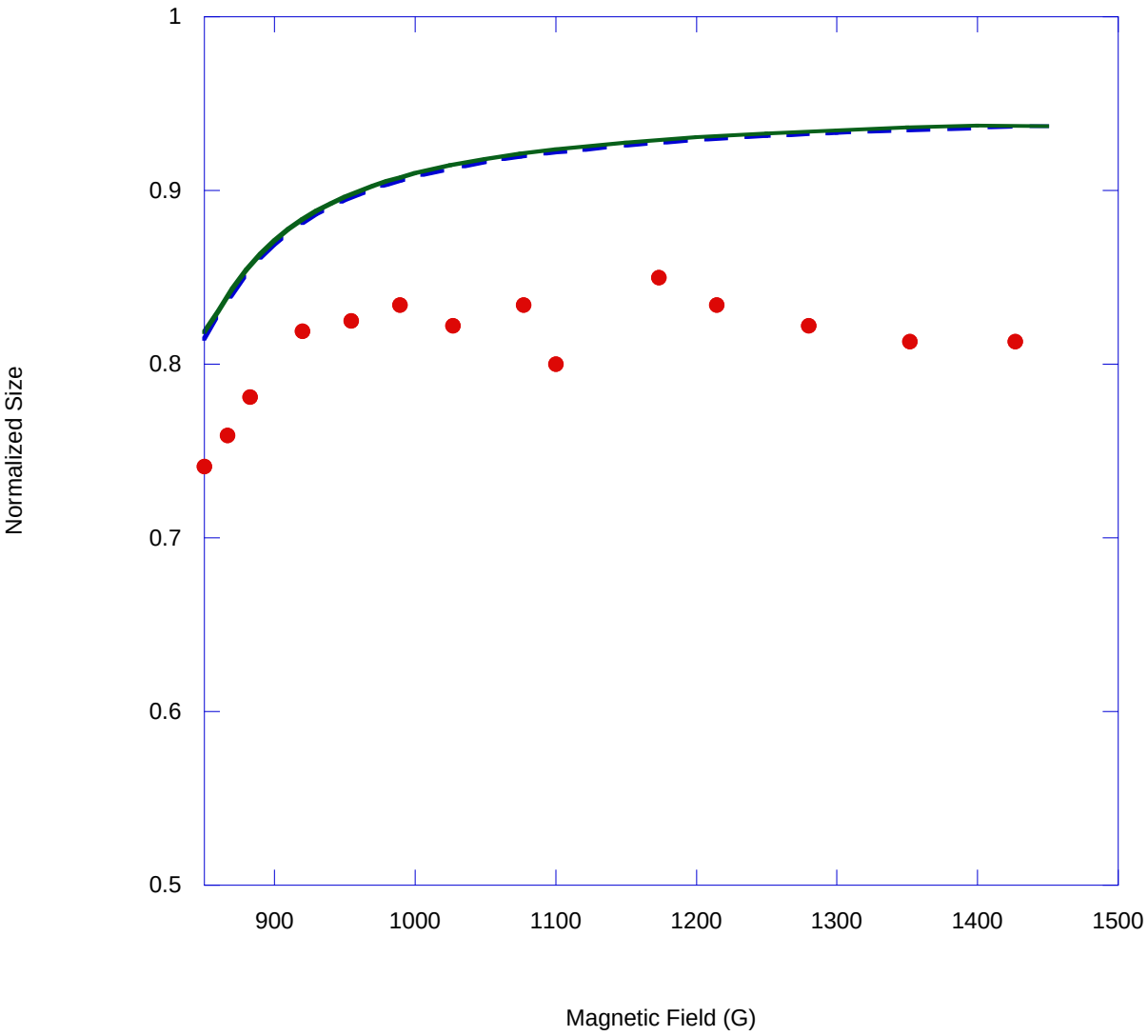

Fig. 3. Axial cloud size of strongly interacting ^6Li atoms after normalization to a non-interacting Fermi gas with $N = 4 \times 10^5$ atoms as a function of the magnetic field B [32]. The trap parameters are $\omega_\perp = 2\pi \times 640$Hz, $\omega_z = 2\pi(600B/kG + 32)^{1/2}$Hz. The solid line and dashed line represent the results of theoretical calculation that includes the OWD or uses the TF approximation for the kinetic energy density, respectively. The circular dots indicate experimental data from the Innsbruck group [11].

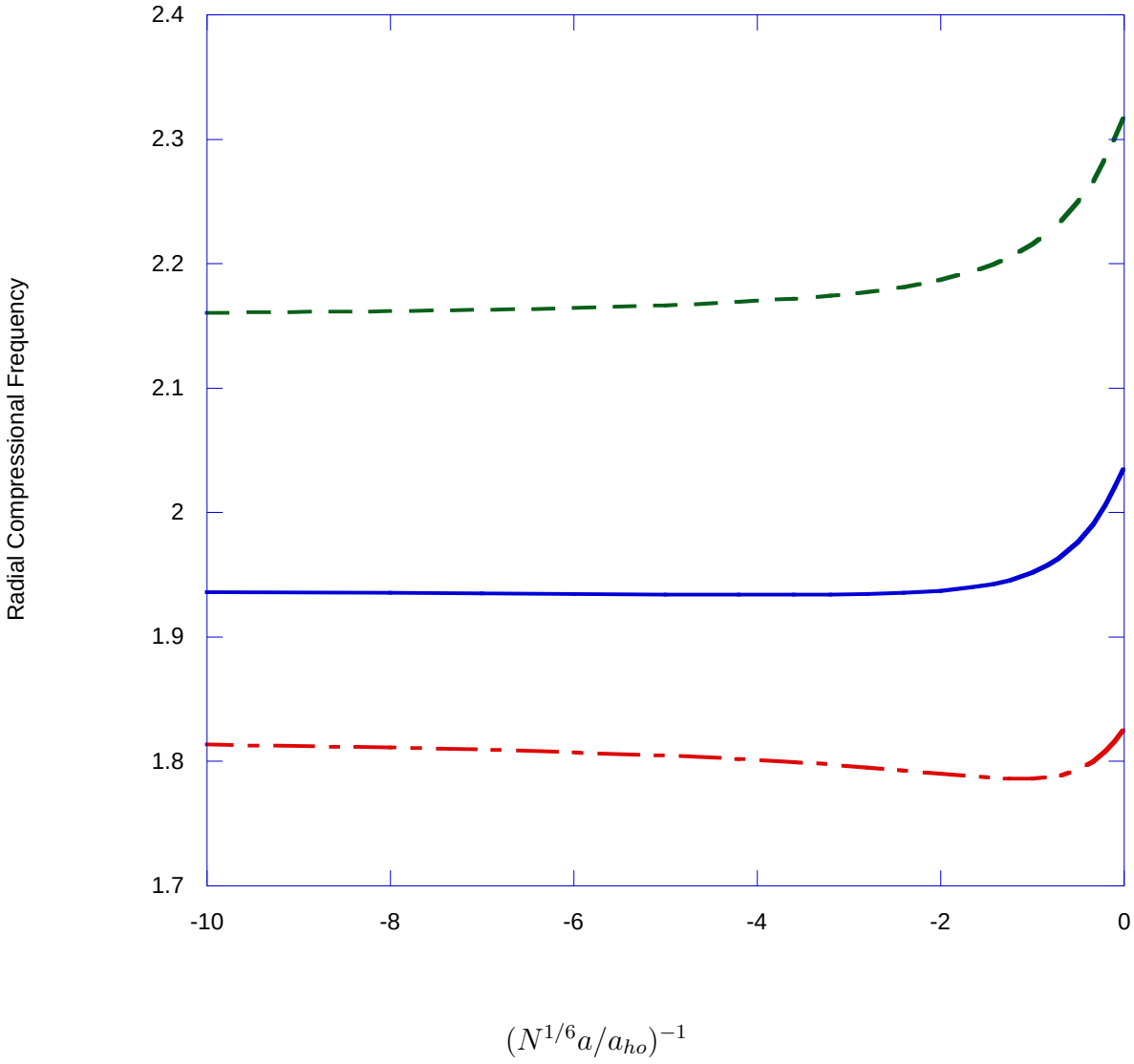

Fig. 4. Radial compressional frequency, ω_{rad}, of the cloud of the $N = 10^4$ fermions (solid line) and $N = 10^3$ fermions (dashed line) in unit of $\omega_\perp$ as a function of the dimensional parameter $(N^{1/6}a/a_{ho})^{-1}$. The trap parameter λ is assumed to be equal to 10^{-2}. The lower line (dashed-dotted line) represents the results in the hydrodynamic approximation, Eqs. (1) and (2), in which ω_{rad} is independent of N for a fixed $(N^{1/6}a/a_{ho})^{-1}$.

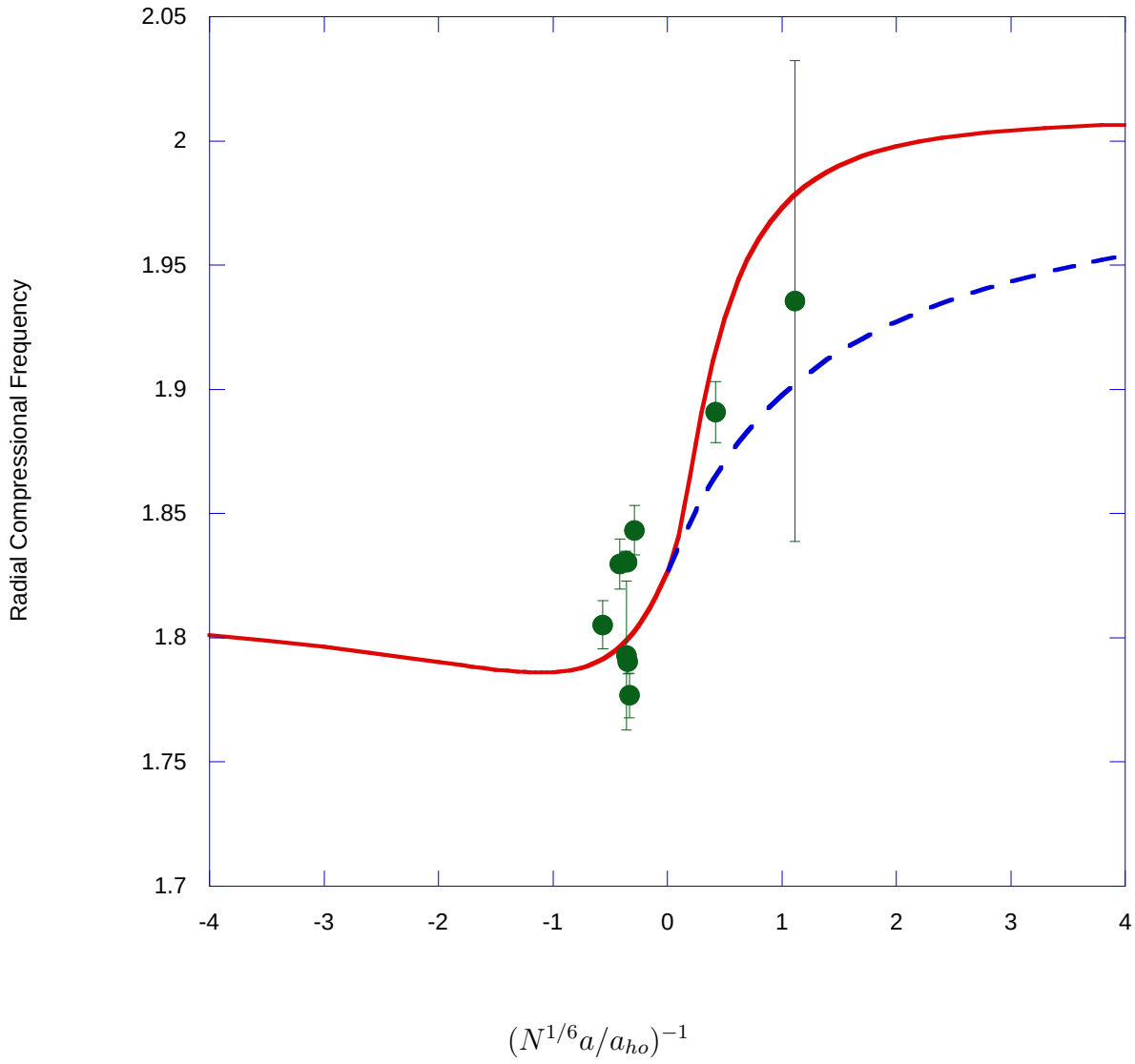

Fig.5. The radial compressional frequency as a function of $(N^{1/6}a/a_{ho})^{-1}$. The solid line and the dashed line represent the results calculated using the [2/2] Padé approximation with $a_m = 0.6a$ and $a_m = 2a$, respectively. The solid circles with error bars are the experimental results given by the Duke University group [1].

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$3^{4/3}/4 \approx 1.08169$ (relative error is less than 0.3%).

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